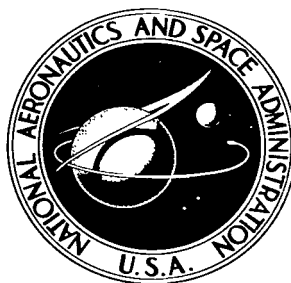


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SELF-STARTING MULTISTEP METHODS FOR THE NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

by William A. Mersman

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Moffett Field, Calif.





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SELF-STARTING MULTISTEP METHODS FOR THE NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

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SUMMARY

Classical, multistep, predictor-corrector procedures for the numerical integration of systems of ordinary differential equations are generalized to provide compatible, self-starting methods. Explicit algorithms and tables of numerical coefficients are presented.

INTRODUCTION

The numerical integration of systems of ordinary differential equations on modern automatic computers is usually accomplished by means of so-called multistep methods, particularly the predictor-corrector methods associated with the names Adams, Bashforth, Moulton, Störmer, and Cowell. It is usually assumed that these methods are not self-starting, and recourse is had to single-step methods like that of Runge-Kutta to obtain starting values. This leads to cumbersome computer programs requiring what amounts to unessential tallying to determine whether enough starting values have been obtained.

The purpose of the present report is to derive simple generalizations of the classical predictor-corrector formulas that immediately yield compatible self-starting procedures that produce all the required backward differences directly from the initial conditions.

STATEMENT OF THE PROBLEM

The problem is to devise a self-starting, multistep procedure for the numerical solution of the initial value problem

$$\left. \begin{aligned} \frac{dx}{dt} &= y \\ \frac{dy}{dt} &= f(x, y, t) \end{aligned} \right\} \quad (1)$$

$$\left. \begin{aligned} x(t_0) &= x_0 \\ y(t_0) &= y_0 \end{aligned} \right\} \quad (2)$$

at the discrete, equally spaced points t_n , $n = 1, 2, 3, \dots$. The variables x , y , and f are vectors, all of the same (finite) dimension.

Let the common interval of the independent variable be denoted by h , so that

$$t_n = t_0 + nh$$

and introduce the usual notation

$$x_n = x(t_n)$$

$$y_n = y(t_n)$$

$$f_n = f(x_n, y_n, t_n)$$

The index, n , will be restricted to integral values, usually positive, although negative values will be introduced in some of the starting procedures to be discussed later.

The general problem, then, is to devise algorithms for calculating x_n , y_n , f_n , for $n = 1, 2, 3, \dots$, given simply the differential equations (1) and the initial values (2). The theory for first-order systems is obtained by ignoring the variable, x , throughout the general theory.

The procedure to be used is the conventional one of approximating the function, f , by a polynomial in t of degree q . The problem is then split into two: the forward integration problem and the starting problem.

The Forward Integration Problem

The problem of integrating forward one step will be solved by means of backward difference formulas of the Adams type. Here it is assumed that t_n , x_n , y_n , f_n , and the first q backward differences of f_n :

$$\left. \begin{aligned} \nabla^0 f_n &= f_n \\ \nabla f_n &= f_n - f_{n-1} \\ \nabla^k f_n &= \nabla^{k-1} f_n - \nabla^{k-1} f_{n-1} \\ k &= 1(1)q \end{aligned} \right\} \quad (3)$$

are known. Several algorithms will be derived for computing all these quantities at $t = t_{n+1}$.

The Starting Problem

Before the forward integration algorithms can be applied, it is necessary to compute initial values of the backward differences of f at some point, preferably at $t = t_0$. This will be done by developing iterative algorithms

for the backward calculation of x_{-n} , y_{-n} , f_{-n} at $n = 1(1)q$, from which the backward differences of f_0 are easily calculated.

It sometimes happens that the initial values lie near a singularity. In this case the backward starter may fail. For this reason, iterative forward starters will also be derived for the calculation of x_n , y_n , f_n , at $n = 1(1)q$.

In either case the final "output" of the starting procedure will be x_0 , y_0 , f_0 , and the first q backward differences of f_0 , so that the starter will be compatible with the forward integration procedures.

In the following section the basic backward difference equations will be derived. These are generalizations of the equations usually ascribed to Adams, Bashforth, Moulton, Störmer, and Cowell (ref. 1, chs. 5 and 6). It is the generalization of the classical formulas that makes self-starting procedures possible.

GENERALIZED BACKWARD DIFFERENCE EQUATIONS

Normal Form

The basic difference equations, relating ∇y , ∇x , and $\nabla^2 x$ at $t = t_j$ to f and its backward differences at $t = t_n$, both j and n being arbitrary, are

$$\nabla y_j = h \sum_{k=0}^{\infty} \gamma_{n-j,k} \nabla^k f_n \quad (4)$$

$$\nabla^2 x_j = h^2 \sum_{k=0}^{\infty} \sigma_{n-j,k} \nabla^k f_n \quad (5)$$

$$\nabla x_j = h y_n + h^2 \sum_{k=0}^{\infty} (\sigma_{n-j,k+1} - \gamma_{0,k+1}) \nabla^k f_n \quad (6)$$

These are written formally as infinite series to simplify certain index manipulations. They terminate and are exact whenever f is a polynomial in t .

The proof is a straightforward generalization of Henrici's (ref. 1, pp. 191-194 and 290-293). Write y_j as a Taylor's series with remainder centered at t_{j-1} (ref. 2, p. 95):

$$y_j = y_{j-1} + h \int_0^1 f(t_{j-1} + \tau h) d\tau$$

Now note that

$$t_{j-1} + \tau h = t_n - (n - j + 1 - \tau)h$$

Approximating f by means of Newton's interpolating polynomial (ref. 1, pp. 190-191)

$$f(t_n - sh) = \sum_{k=0}^{\infty} (-1)^k \binom{s}{k} \nabla^k f_n$$

where the symbol

$$\binom{s}{k} = \frac{\Gamma(s+1)}{k! \Gamma(s+1-k)}$$

yields equation (4), with γ given by

$$\gamma_{p,k} = (-1)^k \int_0^1 \binom{p+1-\tau}{k} d\tau \quad (7)$$

Equation (5) is obtained similarly by writing the Taylor's series for x_j and x_{j-2} centered at t_{j-1}

$$x_j = x_{j-1} + hy_{j-1} + h^2 \int_0^1 (1-\tau) f(t_{j-1} + \tau h) d\tau$$

$$x_{j-2} = x_{j-1} - hy_{j-1} + h^2 \int_0^1 (1-\tau) f(t_{j-1} - \tau h) d\tau$$

adding and inserting Newton's interpolating polynomial yields equation (5), with σ given by

$$\sigma_{p,k} = (-1)^k \int_0^1 (1-\tau) \left[\binom{p+1-\tau}{k} + \binom{p+1+\tau}{k} \right] d\tau \quad (8)$$

Before deriving equation (6) it is convenient to discuss equations (4) and (5) and some of the properties of γ and σ .

Equation (4) with $j = n+1$ is the Adams-Bashforth predictor (ref. 1, pp. 192-193). Henrici uses the notation

$$\gamma_k = \gamma_{-1,k}$$

Equation (4) with $j = n$ is the Adams-Moulton corrector (ref. 1, pp. 194-195). Henrici uses the notation

$$\gamma_k^* = \gamma_{0,k}$$

Equation (5) with $j = n+1$ is the Störmer predictor (ref. 1, pp. 291-292). Henrici uses the notation

$$\sigma_k = \sigma_{-1,k}$$

Equation (5) with $j = n$ is the Cowell corrector (ref. 1, pp. 292-293). Henrici uses the notation

$$\sigma_k^* = \sigma_{0,k}$$

As will be seen later, equations (4) to (6) with $j = n - q(1)n - 1$ form the basis for the self-starting procedures to be developed.

The most important property of γ and σ is that each row is the first backward difference of the preceding row:

$$\left. \begin{aligned} \gamma_{p+1,k} &= \gamma_{p,k} - \gamma_{p,k-1} \\ \sigma_{p+1,k} &= \sigma_{p,k} - \sigma_{p,k-1} \end{aligned} \right\} k \geq 1 \quad (9)$$

while $\gamma_{p,0} = \sigma_{p,0} = 1$. These follow immediately from the definitions, equations (7), (8), and the well-known recurrence relation for the binomial coefficients:

$$\binom{\alpha + 1}{k} = \binom{\alpha}{k} + \binom{\alpha}{k-1}$$

Equations (9) can be rearranged in the useful form

$$\left. \begin{aligned} \nabla_j \gamma_{n-j,k+1} &= \gamma_{n-j,k} \\ \nabla_j \sigma_{n-j,k+1} &= \sigma_{n-j,k} \end{aligned} \right\} \quad (10)$$

where the subscript on ∇_j is used to emphasize that ∇ here operates on j , not on n or k .

The tables of γ and σ at the end of the report were computed by means of the definitions, equations (7) and (8), for the first row ($p = -1$), and the difference equations (9) for subsequent rows.

To return to the derivation of equation (6), note first that x bears the same relation to y as y does to f . Hence, we can write equation (4) in the transliterated form

$$\nabla x_j = h \sum_{m=0}^{\infty} \gamma_{n-j,m} \nabla^m y_n \quad (4a)$$

Writing equation (4) with $j = n$ gives

$$\nabla y_n = h \sum_{r=0}^{\infty} \gamma_{0,r} \nabla^r f_n$$

and taking the $(m-1)$ st backward difference gives

$$\nabla^m y_n = h \sum_{r=0}^{\infty} \gamma_{0,r} \nabla^{m+r-1} f_n$$

Substituting in equation (4a) and rearranging gives

$$\nabla x_j = hy_n + h^2 \sum_{k=0}^{\infty} \sum_{r=0}^k \gamma_{0,r} \gamma_{n-j,k+1-r} \nabla^k f_n \quad (11)$$

Applying the backward difference operator ∇_j and using equations (10) gives

$$\nabla^2 x_j = h^2 \sum_{k=0}^{\infty} \sum_{n=0}^k \gamma_{0,r} \gamma_{n-j,k-r} \nabla^k f_n$$

Comparison with equation (5) gives the important identity

$$\sigma_{p,k} = \sum_{r=0}^k \gamma_{0,r} \gamma_{p,k-r} \quad (12)$$

Hence,

$$\sum_{r=0}^k \gamma_{0,r} \gamma_{p,k+1-r} = \sigma_{p,k+1} - \gamma_{0,k+1}$$

and this reduces equation (11) to equation (6). Q.E.D.

Equation (12) constitutes a valuable check on the tables of γ and σ and has been used. In addition, for small values of k , it is convenient to have the explicit formulas

$$\left. \begin{aligned} \gamma_{p,0} &= 1 \\ \gamma_{p,1} &= -p - \frac{1}{2} \\ \gamma_{p,2} &= \frac{1}{2} p^2 - \frac{1}{12} \end{aligned} \right\} \quad (13)$$

$$\left. \begin{aligned} \sigma_{p,0} &= 1 \\ \sigma_{p,1} &= -p - 1 \\ \sigma_{p,2} &= \frac{p(p+1)}{2} + \frac{1}{12} \end{aligned} \right\} \quad (14)$$

Equation (6), with $j = n+1$ or n , constitutes a new predictor-corrector scheme, to be discussed later, which appears to have some advantages over the Störmer-Cowell scheme of equation (5). For $j = n - q(1)n - 1$, equation (6), like equations (4) and (5), forms the basis for an iterative starter.

This completes the derivation of the basic backward difference equations in the normal form. Closely related to these are similar equations using the

first and second sums. Astronomers have long used these concepts (ref. 3), and further confirmation of their effectiveness is offered by Henrici (ref. 1, pp. 327-339). These summed forms will be derived in the next section.

Summed Form

The basic difference equations, in the summed form, relating x and y at $t = t_j$ to f , its backward differences and its backward sums at $t = t_n$, both j and n being arbitrary, are

$$\left. \begin{aligned} y_j &= A_n + h \sum_{k=0}^{\infty} \gamma_{n-j, k+1} \nabla^k f_n \\ x_j &= B_n + (j - n - 1)hA_n + h^2 \sum_{k=0}^{\infty} \sigma_{n-j, k+2} \nabla^k f_n \end{aligned} \right\} \quad (15)$$

where the backward sums A_n and B_n are defined by these same equations with $j = n$:

$$\left. \begin{aligned} A_n &= y_n - h \sum_{k=0}^{\infty} \gamma_{0, k+1} \nabla^k f_n \\ B_n &= x_n + hA_n - h^2 \sum_{k=0}^{\infty} \sigma_{0, k+2} \nabla^k f_n \end{aligned} \right\} \quad (16)$$

The names first and second sum for A_n and B_n , respectively, are justified by the property

$$\left. \begin{aligned} \nabla A_n &= hf_n \\ \nabla B_n &= hA_n \end{aligned} \right\} \quad (17)$$

The proof is quite straightforward. Replace the coefficient, γ , in equation (4) by its equivalent value from equations (10):

$$\nabla_j y_j = \nabla_j \left(h \sum_{k=0}^{\infty} \gamma_{n-j, k+1} \nabla^k f_n \right)$$

where, again, the subscript j is affixed to ∇ to emphasize that the operator, especially in the right member, acts on j rather than n or k . This is a simple, linear difference equation whose solution is obviously the first of equations (15), in which A_n is an arbitrary constant vector, independent of j , whose value is determined by setting $j = n$, equations (16).

If y_n is now eliminated from equation (6) by means of the first of equations (16), and if the coefficient, σ , is replaced by means of equations (10), the result is again a simple, linear difference equation:

$$\nabla_j x_j = hA_n + \nabla_j \left(h^2 \sum_{k=0}^{\infty} \sigma_{n-j,k} \nabla^k f_n \right)$$

whose solution is clearly the second of equations (15), where B_n is another arbitrary constant vector independent of j , whose value is determined by setting $j = n$ (eqs.(16)).

Equations (17) follow immediately from equations (16) on taking the backward difference and applying equations (4) and (6) with $j = n$.

As will be seen in later sections, equations (16) will be used only once, in connection with the starting procedure, to obtain initial values, A_0 and B_0 , of the first and second sums. Subsequently, equations (15) with $j = n+1$ will yield the summed versions of the Adams-Bashforth and Störmer predictors, while equations (15) and (17), with n replaced by $n+1$ and $j = n+1$, will yield the summed versions of the Adams-Moulton and Cowell correctors.

Before discussing starting procedures, it is necessary to convert the basic difference equations (4), (5), (6), (15), and (16) to the backward ordinate form, in which earlier values of f are used rather than its backward differences.

GENERALIZED BACKWARD ORDINATE EQUATIONS

The backward difference equations of previous sections have been written formally as infinite series merely for manipulative convenience. In practice, it is assumed that f is approximated by a polynomial in t of degree q , say, and the series are all truncated at $k = q$. If, then, the backward differences in equations (15) and (16) are eliminated by means of the well-known identity (ref. 1, p. 190)

$$\nabla^k f_n = \sum_{m=0}^k (-1)^m \binom{k}{m} f_{n-m}$$

and the order of summation is reversed in the resulting double sums, the following backward ordinate equations are obtained in summed form:

$$\left. \begin{aligned} y_j &= A_n + h \sum_{m=0}^q \gamma_{q,n-j,m} f_{n-m} \\ x_j &= B_n + (j - n - 1)hA_n + h^2 \sum_{m=0}^q \sigma_{q,n-j,m} f_{n-m} \end{aligned} \right\} \quad (18)$$

where the coefficients γ and σ are

$$\left. \begin{aligned} \gamma_{q,p,m} &= (-1)^m \sum_{k=m}^q \binom{k}{m} \gamma_{p,k+1} \\ \sigma_{q,p,m} &= (-1)^m \sum_{k=m}^q \binom{k}{m} \sigma_{p,k+2} \end{aligned} \right\} \quad (19)$$

Again the sums A_n and B_n are given by setting $j = n$:

$$\left. \begin{aligned} A_n &= y_n - h \sum_{m=0}^q \gamma_{q,o,m} m^n \\ B_n &= x_n + h A_n - h^2 \sum_{m=0}^q \sigma_{q,o,m} m^n \end{aligned} \right\} \quad (20)$$

Eliminating A_n and B_n from equations (18) and (20) then gives the normal form of the backward ordinate equations:

$$\left. \begin{aligned} y_j &= y_n - h \sum_{m=0}^q \alpha_{q,n-j,m} m^n \\ x_j &= x_n - (n-j) h y_n + h^2 \sum_{m=0}^q \beta_{q,n-j,m} m^n \end{aligned} \right\} \quad (21)$$

where the coefficients α and β are

$$\left. \begin{aligned} \alpha_{q,p,m} &= \gamma_{q,o,m} - \gamma_{q,p,m} \\ \beta_{q,p,m} &= \sigma_{q,p,m} - \sigma_{q,o,m} + p \gamma_{q,o,m} \end{aligned} \right\} \quad (22)$$

The tables of γ , σ , α , and β at the end of the report were computed using equations (19) and (22) together with the easily proved relations:

$$\begin{aligned} \gamma_{q,p,o} &= \gamma_{p-1,q+1} - 1 \\ \sigma_{q,p,o} &= \sigma_{p-1,q+2} + p + 1 \\ \gamma_{q,p,q} &= (-1)^q \gamma_{p,q+1} \\ \sigma_{q,p,q} &= (-1)^q \sigma_{p,q+2} \\ \gamma_{q+1,p,m} &= \gamma_{q,p,m} + (-1)^m \binom{q+1}{m} \gamma_{p,q+2} \\ \sigma_{q+1,p,m} &= \sigma_{q,p,m} + (-1)^m \binom{q+1}{m} \sigma_{p,q+3} \end{aligned}$$

Taking $f(t) = t^r$ in equations (21), $r = 0(1)q$, gives the identities

$$\sum_{m=0}^q m^r \alpha_{q,p,m} = \frac{p^{r+1}}{r+1}, \quad \sum_{m=0}^q \gamma_{q,p,m} = \gamma_{p,1}$$

$$\sum_{m=0}^q m^r \beta_{q,p,m} = \frac{p^{r+2}}{(r+1)(r+2)}, \quad \sum_{m=0}^q \sigma_{q,p,m} = \sigma_{p,2}$$

which were used as a final check on the tables.

All the basic formulas, summed and normal, in backward difference and backward ordinate forms, have now been derived. The remaining sections of the report are devoted to the presentation of general and specific algorithms for starting and continuing the integration.

BACKWARD STARTING ALGORITHMS

A backward starting algorithm is one that produces the backward differences of f_0 , up to order q , given merely the initial conditions, equations (2), and, of course, the differential equations (1). This is equivalent to an algorithm that will produce backward values of the ordinates, f_{-p} , for $p = 1(1)q$; it is then a simple matter to obtain the backward differences at f_0 . (See the appendix for details.)

The desired algorithm, in normal form, is implicitly contained in equations (21) with $n = 0$, $j = -p$:

$$\left. \begin{aligned} y_{-p} &= y_0 - h \sum_{m=0}^q \alpha_{q,p,m} f_{-m} \\ x_{-p} &= x_0 - phy_0 + h^2 \sum_{m=0}^q \beta_{q,p,m} f_{-m} \\ f_{-p} &= f(t_0 - ph, x_{-p}, y_{-p}) \end{aligned} \right\} \quad (23)$$

for $p = 1(1)q$. This is a set of $3q$ implicit equations for the $3q$ unknowns y_{-p} , x_{-p} , f_{-p} .

If an approximate solution is known, an improved solution is readily obtained by iterating equations (23); inserting "old" values in the right members produces "new" values in the left members. Collatz (ref. 4, pp. 99-101) exhibits the α for $q = 2, 3$ and discusses the convergence of the iteration, but does not derive the general formulas. Two methods of obtaining an initial approximation will now be given.

Bootstrap Starter

Since only one value of f , namely f_0 , is known initially, the simplest possible procedure is to take $q = 0$ in equations (23). Setting $p = 1$ gives the "predicted" values of x , y , and f at t_{-1} . Then setting $q = 1$, $p = 1$, gives corrected values. Keeping $q = 1$ and now setting $p = 2$, gives predicted values at t_{-2} . This bootstrapping procedure can be repeated until the desired value of q is reached. The explicit algorithm is

$$\begin{array}{ll}
 \text{Predictor} & \begin{array}{l} p = 1(1)q \\ y_{-p} = y_0 - h \sum_{m=0}^{p-1} \alpha_{p-1,p,m} f_{-m} \\ x_{-p} = x_0 - phy_0 + h^2 \sum_{m=0}^{p-1} \beta_{p-1,p,m} f_{-m} \\ f_{-p} = f(t_{-p}, x_{-p}, y_{-p}) \end{array} \\
 \text{Multiple corrector} & \begin{array}{l} k = 1(1)p \\ y_{-k} = y_0 - h \sum_{m=0}^p \alpha_{p,k,m} f_{-m} \\ x_{-k} = x_0 - khy_0 + h^2 \sum_{m=0}^p \beta_{p,k,m} f_{-m} \\ f_{-k} = f(t_{-k}, x_{-k}, y_{-k}) \end{array}
 \end{array} \quad (24)$$

Experienced computer programmers will recognize this as a simple, nested DO LOOP.

To make the procedure more tangible, the first few algorithms are written explicitly below:

$$\begin{array}{ll}
 p = 1; \text{ predictor} & \begin{array}{l} y_{-1} = y_0 - hf_0 \\ x_{-1} = x_0 - hy_0 + \frac{h^2}{2} f_0 \\ f_{-1} = f(t_{-1}, x_{-1}, y_{-1}) \end{array} \\
 k = 1; \text{ corrector} & \begin{array}{l} y_{-1} = y_0 - \frac{h}{2} (f_0 + f_{-1}) \\ x_{-1} = x_0 - hy_0 + \frac{h^2}{6} (2f_0 + f_{-1}) \\ f_{-1} = f(t_{-1}, x_{-1}, y_{-1}) \end{array}
 \end{array}$$

$$p = 2; \text{ predictor } y_{-2} = y_0 - 2hf_{-1}$$

$$x_{-2} = x_0 - 2hy_0 + \frac{h^2}{3} (2f_0 + 4f_{-1})$$

$$f_{-2} = f(t_{-2}, x_{-2}, y_{-2})$$

$$\text{Multiple corrector } \begin{cases} y_{-1} = y_0 - \frac{h}{12} (5f_0 + 8f_{-1} - f_{-2}) \\ k = 1 \begin{cases} x_{-1} = x_0 - hy_0 + \frac{h^2}{24} (7f_0 + 6f_{-1} - f_{-2}) \\ f_{-1} = f(t_{-1}, x_{-1}, y_{-1}) \end{cases} \end{cases}$$

$$k = 2 \begin{cases} y_{-2} = y_0 - \frac{h}{3} (f_0 + 4f_{-1} + f_{-2}) \\ x_{-2} = x_0 - 2hy_0 + \frac{h^2}{3} (2f_0 + 4f_{-1}) \\ f_{-2} = f(t_{-2}, x_{-2}, y_{-2}) \end{cases}$$

$$p = 3; \text{ predictor } y_{-3} = y_0 - \frac{h}{4} (3f_0 + 9f_{-2})$$

$$x_{-3} = x_0 - 3hy_0 + \frac{h^2}{8} (9f_0 + 18f_{-1} + 9f_{-2})$$

$$f_{-3} = f(t_{-3}, x_{-3}, y_{-3})$$

$$\text{Multiple corrector } \begin{cases} y_{-1} = y_0 - \frac{h}{24} (9f_0 + 19f_{-1} - 5f_{-2} + f_{-3}) \\ k = 1 \begin{cases} x_{-1} = x_0 - hy_0 + \frac{h^2}{360} (97f_0 + 114f_{-1} - 39f_{-2} + 8f_{-3}) \\ f_{-1} = f(t_{-1}, x_{-1}, y_{-1}) \end{cases} \end{cases}$$

$$k = 2 \begin{cases} y_{-2} = y_0 - \frac{h}{3} (f_0 + 4f_{-1} + f_{-2}) \\ x_{-2} = x_0 - 2hy_0 + \frac{h^2}{45} (28f_0 + 66f_{-1} - 6f_{-2} + 2f_{-3}) \\ f_{-2} = f(t_{-2}, x_{-2}, y_{-2}) \end{cases}$$

$$k = 3 \begin{cases} y_{-3} = y_0 - \frac{h}{8} (3f_0 + 9f_{-1} + 9f_{-2} + 3f_{-3}) \\ x_{-3} = x_0 - 3hy_0 + \frac{h^2}{360} (351f_0 + 972f_{-1} + 243f_{-2} + 54f_{-3}) \\ f_{-3} = f(t_{-3}, x_{-3}, y_{-3}) \end{cases}$$

The bootstrap starter seems to be quite efficient in practice, but it is awkward and space-consuming when programmed for automatic computers, because of the multiplicity of matrices and algorithms required. This suggests the following logically simpler method.

Iterated Starter

The bootstrap starter is essentially an efficient method of obtaining first approximations for use in the right members of equations (23), which are then iterated. A logically simpler, but less efficient method is to initialize by setting $f_{-m} = f_0$, $m = 1(1)q$, in the right members, and then iterate the single set of equations (23).

Backward Starter, Summed Form

Starting with equations (18) and (20), instead of (23) and again setting $n = 0$, $j = -p$ gives the implicit, summed form of the backward starter:

$$\left. \begin{aligned}
 p &= 1(1)q \\
 y_{-p} &= A_0 + h \sum_{m=0}^q \gamma_{q,p,m} f_{-m} \\
 x_{-p} &= B_0 - (p+1)hA_0 + h^2 \sum_{m=0}^q \sigma_{q,p,m} f_{-m} \\
 f_{-p} &= f(t_{-p}, x_{-p}, y_{-p}) \\
 A_0 &= y_0 - h \sum_{m=0}^q \gamma_{q,0,m} f_{-m} \\
 B_0 &= x_0 + hA_0 - h^2 \sum_{m=0}^q \sigma_{q,0,m} f_{-m}
 \end{aligned} \right\} \quad (25)$$

Initial values can be obtained by the obvious bootstrap procedure or by starting with $f_{-m} = f_0$, $m = 1(1)q$.

$$\begin{aligned}
 A_0 &= y_0 + \frac{h}{2} f_0 \\
 B_0 &= x_0 + hA_0 - \frac{h^2}{12} f_0 = x_0 + hy_0 + \left(\frac{5}{12}\right) h^2 f_0
 \end{aligned}$$

Equations (25) can then be iterated until they converge.

This algorithm is mentioned mainly for the sake of completeness. The principal reason for introducing the first and second sums is to obtain better control of the accumulated round-off error during a long integration, but this consideration may be irrelevant to a starting procedure.

Before turning to the subject of forward starting procedures, it may be noticed that the backward starter (eqs. (23)) produces the ordinates f_{-p} , $p = 1(1)q$. These are easily converted to backward differences at f_0 (see the

appendix). If summed forms of the forward integration procedure are to be used subsequently, the initial values of A_0 and B_0 are easily computed from equations (16), with $n = 0$. Thus even here there is no compulsion to use the summed form of the starter.

FORWARD STARTING ALGORITHMS

The derivation of forward starting algorithms is almost trivial. Each of the backward starters discussed previously becomes a forward starter by means of the simple transformation

$$h \rightarrow -h$$

$$x_{-m} \rightarrow x_m$$

$$y_{-m} \rightarrow y_m$$

$$f_{-m} \rightarrow f_m$$

This produces the forward ordinates, f_m , $m = 0(1)q$.

The conversion to backward differences at t_q is straightforward. However, to do this on an automatic computer would involve either losing all information at the points between t_0 and t_q , or else increasing the storage requirements excessively. Furthermore, either choice leads to a procedure that is different, in its external appearance and mode of usage, from the backward starter.

A preferable procedure is to compute the backward difference table at t_q and then extend it back to t_0 by holding $\nabla^q f$ constant; this, of course, is consistent with the starting procedure. This is easily done, and programming details are given in the appendix.

Choosing the latter alternative provides computer programmers with a battery of starting procedures, forward or backward, bootstrap or iterative, in normal or summed form, with identical external appearance. In every case the input data consist of the initial conditions, and the output data consist of the table of backward differences (and sums) at the initial point, in a form compatible with the forward integration procedures to be discussed next.

PREDICTOR-CORRECTOR ALGORITHMS FOR FORWARD INTEGRATION

The purpose of this section is to present a variety of algorithms for the forward integration from t_n to t_{n+1} . Specifically, it is assumed that the input consists of t_n , x_n , y_n , f_n , and the first q backward differences of f_n , together with the sums A_n and B_n when appropriate. The output is to be

the same list of quantities at t_{n+1} . The combination of any of these algorithms with any of the starters provides the complete solution of the initial-value problem.

All the algorithms to be presented involve the use of a predictor followed by a corrector, requiring two calculations of $f(x,y,t)$. Conflicting philosophies regarding the need for a corrector can be found in references 3 and 5. The general consensus among automatic computer users seems to favor the use of one corrector. In the algorithms given below the user can, of course, omit the corrector if he chooses.

The backward difference equations (4) through (6) and (15) through (17) give predictor formulas when $j = n + 1$. Taking $j = n$ and then replacing n by $n + 1$ yields corrector formulas. In every case, if both predictor and corrector are truncated at the same value $k = q$, then subtracting the predictor from the corrector and using the recurrence relations (eqs. (9)) for the coefficients γ and σ gives a shorter formula for the corrector.

Throughout, predicted values are indicated by an asterisk (*).

Normal Form

First-order system.— The Adams-Bashforth predictor is

$$y_{n+1}^* = y_n + h \sum_{k=0}^q \gamma_{-1,k} \nabla^k f_n \quad (26)$$

and the Adams-Moulton corrector is

$$y_{n+1} = y_{n+1}^* + h \gamma_{-1,q} \nabla^{q+1} f_{n+1}^* \quad (27)$$

Simple second-order system.— If the first derivative, y , does not occur in the differential equation and is not required, the formulas for x are:

Störmer predictor

$$x_{n+1}^* = 2x_n - x_{n-1} + h^2 \sum_{k=0}^q \sigma_{-1,k} \nabla^k f_n \quad (28)$$

Cowell corrector

$$x_{n+1} = x_{n+1}^* + h^2 \sigma_{-1,q} \nabla^{q+1} f_{n+1}^* \quad (29)$$

General second-order system.— When the first derivation, y , is present, equations (4) and (6) yield the predictor

$$\left. \begin{aligned} y_{n+1}^* &= y_n + h \sum_{k=0}^q \gamma_{-1,k} \nabla^k f_n \\ x_{n+1}^* &= x_n + h y_{n+1}^* + h^2 \sum_{k=0}^q (\sigma_{-1,k+1} - \gamma_{-1,k+1}) \nabla^k f_n \end{aligned} \right\} \quad (30)$$

and the corrector

$$\left. \begin{aligned} y_{n+1} &= y_{n+1}^* + h \gamma_{-1,q} \nabla^{q+1} f_{n+1}^* \\ x_{n+1} &= x_{n+1}^* + h^2 (\sigma_{-1,q+1} - \gamma_{0,q+1}) \nabla^{q+1} f_{n+1}^* \end{aligned} \right\} \quad (31)$$

Summed Form

The predictor is

$$\left. \begin{aligned} y_{n+1}^* &= A_n + h \sum_{k=0}^q \gamma_{-1,k+1} \nabla^k f_n \\ x_{n+1}^* &= B_n + h^2 \sum_{k=0}^q \sigma_{-1,k+2} \nabla^k f_n \end{aligned} \right\} \quad (32)$$

The corrector is

$$\left. \begin{aligned} y_{n+1} &= y_{n+1}^* + h \gamma_{-1,q+1} \nabla^{q+1} f_{n+1}^* \\ x_{n+1} &= x_{n+1}^* + h^2 \sigma_{-1,q+2} \nabla^{q+1} f_{n+1}^* \end{aligned} \right\} \quad (33)$$

and, of course,

$$\left. \begin{aligned} A_{n+1} &= A_n + h f_{n+1} \\ B_{n+1} &= B_n + h A_{n+1} \end{aligned} \right\} \quad (34)$$

In all these predictor-corrector algorithms, the calculation of the difference table is facilitated by noting that, on defining

$$\epsilon = f_{n+1} - f_{n+1}^*$$

the differences are

$$\nabla^k f_{n+1} = \nabla^k f_{n+1}^* + \epsilon, \quad k = 1(1)q$$

(see ref. 1, p. 196). The predicted differences, $\nabla^k f_{n+1}^*$, are obtained, of course, directly from the definition:

$$\nabla f_{n+1}^* = f_{n+1}^* - f_n$$

$$\nabla^{k+1} f_{n+1}^* = \nabla^k f_{n+1}^* - \nabla^k f_n, \quad k = 1(1)q$$

CONCLUDING REMARKS

The present report displays a variety of algorithms for starting and continuing the numerical integration of systems of ordinary differential equations. The exhaustive testing of these algorithms, for the purpose of comparing their effectiveness, would be an expensive process. Fortunately, a great deal of relevant experience has been obtained in recent years in computing installations throughout the world. In the present writer's opinion the best compromise between the conflicting desiderata of speed, accuracy, and programming compactness can be achieved by the following choice:

- (1) Use the fourth-order methods for first-order equations, sixth-order methods for second-order equations ($q = 4, 6$, respectively).
- (2) Use the iterated starter, iterated eight times.
- (3) Use the summed form of the predictor-corrector algorithm, in backward difference form.
- (4) Carry four extra significant decimal digits, in floating-point form, to control round-off errors.

The effectiveness of the summed form of the predictor-corrector algorithms has long been known to astronomers (ref. 3), and additional evidence is furnished by Henrici (ref. 1, pp. 336-339). The iterated starter is somewhat less efficient than the bootstrap version, but is far simpler to program and is much more modest in its storage requirements.

The use of backward differences in the forward integration is preferable to the use of backward ordinates for two reasons: (1) the backward ordinate formula tends to add nearly equal quantities of alternating sign, whereas the backward difference formula adds monotonically decreasing quantities; and (2) the availability of the difference table makes error estimation and automatic adjustment of the interval size a straightforward procedure.

Ames Research Center
National Aeronautics and Space Administration
Moffett Field, Calif., April 19, 1965

APPENDIX

CONVERSION OF ORDINATES TO DIFFERENCES

The calculation of a table of backward differences from a table of ordinates, and its extension in either direction when higher order differences are neglected, is a familiar procedure to computers working with pencil and paper. The programming of such procedures for automatic computers is less familiar, and the purpose of this appendix is to give some typical algorithms in FORTRAN format, the most widely used scientific programming language.

The algorithms exhibited here are written as though x , y , f , A , and B were scalars. When they are vectors, the algorithms are easily generalized by the addition of a second subscript and suitable additional "DO LOOPS" over the range of the second subscript (the dimension of the vectors).

Since the FORTRAN language does not permit subscripts nor indices in loops to assume nonpositive values, certain logical artificialities appear in these algorithms. Experienced programmers should have no difficulty in removing them for other, less restricted, programming languages.

Backward Starter

All the versions of the backward starter discussed in the main body of the report produce the backward ordinates, f_{-p} , $p = 0(1)q$. Suppose these are placed in the array L :

$$L(p + m) = f_{-p}$$

where m is an arbitrary, positive integer. Then the nested DO LOOP

```
      DO          k = 1, q
      [           l = q + 1 - k
      [ DO        j = 1, l
      [           n = m + q - j
      [           L(n + 1) = L(n) - L(n + 1)
```

will yield $\nabla^p f_0$ in $L(p + m)$, $p = 0(1)q$, $q \geq 1$. The structure of the algorithm is illustrated by the following diagram, in which $q = 3$ and $m = 0$ (in violation of the FORTRAN restriction!):

| Initial values | k = 1, l = 3 | k = 2, l = 2 | k = 3, l = 1 |
|------------------------|---|---|---|
| L(3) = f ₋₃ | j = 1, n = 2 L(3) = L(2) - L(3) = f ₋₂ - f ₋₃ = ∇f ₋₂ | j = 1, n = 2 L(3) = L(2) - L(3) = ∇f ₋₁ - ∇f ₋₂ = ∇ ² f ₋₁ | j = 1, n = 2 L(3) = L(2) - L(3) = ∇ ² f ₀ - ∇ ² f ₋₁ = ∇ ³ f ₀ |
| L(2) = f ₋₂ | j = 2, n = 1 L(2) = L(1) - L(2) = f ₋₁ - f ₋₂ = ∇f ₋₁ | j = 2, n = 1 L(2) = L(1) - L(2) = ∇f ₀ - ∇f ₋₁ = ∇ ² f ₀ | |
| L(1) = f ₋₁ | j = 3, n = 0 L(1) = L(0) - L(1) = f ₀ - f ₋₁ = ∇f ₀ | | |
| L(0) = f ₀ | | | |

It is evident from the diagram that increasing q by unity adds one row to each column and adds an additional column on the right with one row.

Forward Starter

All the versions of the forward starter discussed in the main body of the report produce the forward ordinates, f_p, p = 0(1)q. Suppose these are placed in the array L:

$$L(p + m) = f_p$$

Then the nested DO LOOP

```

DO      k = 1, q
  [ DO   l = q + 1 - k
    [ DO   j = 1, l
      [   n = m + q - j
        [   L(n + 1) = L(n + 1) - L(n)

```

will yield $\nabla^p f_p$ in $L(p + m)$, $p = O(1)q$. The diagram illustrates the case $q = 3$, $m = 0$.

| Initial values | $k = 1, l = 3$ | $k = 2, l = 2$ | $k = 3, l = 1$ |
|----------------|---|---|---|
| $L(3) = f_3$ | $j = 1, n = 2$ $L(3) = L(3) - L(2)$ $= f_3 - f_2$ $= \nabla f_3$ | $j = 1, n = 2$ $L(3) = L(3) - L(2)$ $= \nabla f_3 - \nabla f_2$ $= \nabla^2 f_3$ | $j = 1, n = 2$ $L(3) = L(3) - L(2)$ $= \nabla^2 f_3 - \nabla^2 f_2$ $= \nabla^3 f_3$ |
| $L(2) = f_2$ | $j = 2, n = 1$ $L(2) = L(2) - L(1)$ $= f_2 - f_1$ $= \nabla f_2$ | $j = 2, n = 1$ $L(2) = L(2) - L(1)$ $= \nabla f_2 - \nabla f_1$ $= \nabla^2 f_2$ | |
| $L(1) = f_1$ | $j = 3, n = 0$ $L(1) = L(1) - L(0)$ $= f_1 - f_0$ $= \nabla f_1$ | | |
| $L(0) = f_0$ | | | |

To obtain backward differences of f_0 it is necessary to make the assumption that $\nabla^{q+1} f = 0$. Then $\nabla^q f$ is constant:

$$\nabla^q f_p = \nabla^q f_0 = \nabla^q f, \quad p = 1(1)q$$

Then the additional nested DO LOOP

```

      r = q - 1
      DO      k = 1, r
      [      l = q - k
      [      DO      j = 1, l
      [      n = m + q - j
      [      L(n) = L(n) - L(n + 1)

```

yields $\nabla^p f_0$ in $L(p + m)$, $p = O(1)q$, the desired result. The diagram illustrates the case $q = 4$, $m = 0$.

| Initial values | $k = 1, l = 3$ | $k = 2, l = 2$ | $k = 3, l = 1$ |
|-----------------------|---|---|---|
| $L(4) = \nabla^4 f$ | | | |
| $L(3) = \nabla^3 f_3$ | $j = 1, n = 3$ $L(3) = L(3) - L(4)$ $= \nabla^3 f_3 - \nabla^4 f_3$ $= \nabla^3 f_2$ | $j = 1, n = 3$ $L(3) = L(3) - L(4)$ $= \nabla^3 f_2 - \nabla^4 f_2$ $= \nabla^3 f_1$ | $j = 1, n = 3$ $L(3) = L(3) - L(4)$ $= \nabla^3 f_1 - \nabla^4 f_1$ $= \nabla^3 f_0$ |
| $L(2) = \nabla^2 f_2$ | $j = 2, n = 2$ $L(2) = L(2) - L(3)$ $= \nabla^2 f_2 - \nabla^3 f_2$ $= \nabla^2 f_1$ | $j = 2, n = 2$ $L(2) = L(2) - L(3)$ $= \nabla^2 f_1 - \nabla^3 f_1$ $= \nabla^2 f_0$ | |
| $L(1) = \nabla f_1$ | $j = 3, n = 1$ $L(1) = L(1) - L(2)$ $= \nabla f_1 - \nabla^2 f_1$ $= \nabla f_0$ | | |
| $L(0) = f_0$ | | | |

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TABLE I.- $\gamma_{p,k}$

| | γ | 2γ | 12γ | 24γ | 720γ | 1440γ | 60480γ | 120960γ |
|-------|----------|-----------|------------|------------|-------------|--------------|---------------|----------------|
| p/k | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| -1 | 1 | 1 | 5 | 9 | 251 | 475 | 19087 | 36799 |
| 0 | 1 | -1 | -1 | -1 | -19 | -27 | -863 | -1375 |
| 1 | 1 | -3 | 5 | 1 | 11 | 11 | 271 | 351 |
| 2 | 1 | -5 | 23 | -9 | -19 | -11 | -191 | -191 |
| 3 | 1 | -7 | 53 | -55 | 251 | 27 | 271 | 191 |
| 4 | 1 | -9 | 95 | -161 | 1901 | -475 | -863 | -351 |
| 5 | 1 | -11 | 149 | -351 | 6731 | -4277 | 19087 | 1375 |
| 6 | 1 | -13 | 215 | -649 | 17261 | -17739 | 198721 | -36799 |
| 7 | 1 | -15 | 293 | -1079 | 36731 | -52261 | 943759 | -434241 |

TABLE II.- $\sigma_{p,k}$

| | σ | σ | 12σ | 12σ | 240σ | 240σ | 60480σ | 60480σ | 3628800σ |
|-------|----------|----------|------------|------------|-------------|-------------|---------------|---------------|-----------------|
| p/k | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| -1 | 1 | 0 | 1 | 1 | 19 | 18 | 4315 | 4125 | 237671 |
| 0 | 1 | -1 | 1 | 0 | -1 | -1 | -221 | -190 | -9829 |
| 1 | 1 | -2 | 13 | -1 | -1 | 0 | 31 | 31 | 1571 |
| 2 | 1 | -3 | 37 | -14 | 19 | 1 | 31 | 0 | -289 |
| 3 | 1 | -4 | 73 | -51 | 299 | -18 | -221 | -31 | -289 |
| 4 | 1 | -5 | 121 | -124 | 1319 | -317 | 4315 | 190 | 1571 |
| 5 | 1 | -6 | 181 | -245 | 3799 | -1636 | 84199 | -4125 | -9829 |
| 6 | 1 | -7 | 253 | -426 | 8699 | -5435 | 496471 | -88324 | 237671 |
| 7 | 1 | -8 | 337 | -679 | 17219 | -14134 | 1866091 | -584795 | 5537111 |

TABLE III.- $\gamma_{q,p,m}$

| $q = 0: 2\gamma$ | | $q = 1: 12\gamma$ | | $q = 2: 24\gamma$ | | |
|------------------|----|-------------------|-----|-------------------|-----|-----|
| p/m | 0 | 0 | 1 | 0 | 1 | 2 |
| 0 | -1 | -7 | 1 | -15 | 4 | -1 |
| 1 | -3 | -13 | -5 | -25 | -12 | 1 |
| 2 | | -7 | -23 | -23 | -28 | -9 |
| 3 | | | | -33 | 4 | -55 |

| $q = 3: 720\gamma$ | | | | | $q = 4: 1440\gamma$ | | | | |
|--------------------|------|-------|------|-------|---------------------|-------|-------|-------|-------|
| p/m | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 | 4 |
| 0 | -469 | 177 | -87 | 19 | -965 | 462 | -336 | 146 | -27 |
| 1 | -739 | -393 | 63 | -11 | -1467 | -830 | 192 | -66 | 11 |
| 2 | -709 | -783 | -327 | 19 | -1429 | -1522 | -720 | 82 | -11 |
| 3 | -739 | -633 | -897 | -251 | -1451 | -1374 | -1632 | -610 | 27 |
| 4 | -469 | -1743 | 873 | -1901 | -1413 | -1586 | -1104 | -1902 | -475 |
| 5 | | | | | -1915 | 962 | -6336 | 3646 | -4277 |

| $q = 5: 60480\gamma$ | | | | | | |
|----------------------|--------|---------|--------|---------|--------|---------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 |
| 0 | -41393 | 23719 | -22742 | 14762 | -5449 | 863 |
| 1 | -61343 | -36215 | 10774 | -5482 | 1817 | -271 |
| 2 | -60209 | -62969 | -32150 | 5354 | -1417 | 191 |
| 3 | -60671 | -59063 | -65834 | -28330 | 2489 | -271 |
| 4 | -60209 | -62297 | -54998 | -71254 | -24256 | 863 |
| 5 | -61343 | -55031 | -75242 | -37738 | -84199 | -19087 |
| 6 | -41393 | -175865 | 231274 | -456982 | 248567 | -198721 |

| $q = 6: 120960\gamma$ | | | | | | | |
|-----------------------|---------|---------|---------|---------|----------|---------|---------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 0 | -84161 | 55688 | -66109 | 57024 | -31523 | 9976 | -1375 |
| 1 | -122335 | -74536 | 26813 | -17984 | 8899 | -2648 | 351 |
| 2 | -120609 | -124792 | -67165 | 14528 | -5699 | 1528 | -191 |
| 3 | -121151 | -119272 | -128803 | -60480 | 7843 | -1688 | 191 |
| 4 | -120769 | -122488 | -115261 | -135488 | -53795 | 3832 | -351 |
| 5 | -121311 | -118312 | -129859 | -102976 | -147773 | -46424 | 1375 |
| 6 | -119585 | -130936 | -89437 | -177984 | -54851 | -176648 | -36799 |
| 7 | -157759 | 138008 | -903715 | 1198528 | -1465949 | 717928 | -434241 |

TABLE IV.- $\sigma_{q,p,m}$

| q = 0: 12 σ | | q = 1: 12 σ | | q = 2: 240 σ | | |
|--------------------|----|--------------------|----|---------------------|-----|-----|
| p/m | 0 | 0 | 1 | 0 | 1 | 2 |
| 0 | 1 | 1 | 0 | 19 | 2 | -1 |
| 1 | 13 | 12 | 1 | 239 | 22 | -1 |
| 2 | | 23 | 14 | 479 | 242 | 19 |
| 3 | | | | 739 | 422 | 299 |

| q = 3: 240 σ | | | | | q = 4: 60480 σ | | | | |
|---------------------|-----|-----|-----|-----|-----------------------|--------|--------|-------|-------|
| p/m | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 | 4 |
| 0 | 18 | 5 | -4 | 1 | 4315 | 2144 | -2334 | 1136 | -221 |
| 1 | 239 | 22 | -1 | 0 | 60259 | 5420 | -66 | -124 | 31 |
| 2 | 480 | 239 | 22 | -1 | 120991 | 60104 | 5730 | -376 | 31 |
| 3 | 721 | 476 | 245 | 18 | 181471 | 120836 | 60414 | 5420 | -221 |
| 4 | 942 | 793 | 368 | 817 | 241699 | 182576 | 118626 | 62624 | 4315 |
| 5 | | | | | 306715 | 220124 | 225726 | 75476 | 84199 |

| q = 5: 60480 σ | | | | | | |
|-----------------------|--------|--------|--------|--------|-------|-------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 |
| 0 | 4125 | 3094 | -4234 | 3036 | -1171 | 190 |
| 1 | 60290 | 5265 | 244 | -434 | 186 | -31 |
| 2 | 120991 | 60104 | 5730 | -376 | 31 | 0 |
| 3 | 181440 | 120991 | 60104 | 5730 | -376 | 31 |
| 4 | 241889 | 181626 | 120526 | 60724 | 5265 | -190 |
| 5 | 302590 | 240749 | 184476 | 116726 | 63574 | 4125 |
| 6 | 358755 | 327340 | 178874 | 266976 | 54851 | 88324 |

| q = 6: 3628800 σ | | | | | | | |
|-------------------------|----------|----------|----------|----------|----------|---------|---------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 0 | 237671 | 244614 | -401475 | 378740 | -217695 | 70374 | -9829 |
| 1 | 3618971 | 306474 | 38205 | -57460 | 34725 | -11286 | 1571 |
| 2 | 7259171 | 3607974 | 339465 | -16780 | -2475 | 1734 | -289 |
| 3 | 10886111 | 7261194 | 3601905 | 349580 | -26895 | 3594 | -289 |
| 4 | 14514911 | 10888134 | 7255125 | 3612020 | 339465 | -20826 | 1571 |
| 5 | 18145571 | 14503914 | 10921125 | 7200140 | 3667005 | 306474 | -9829 |
| 6 | 21762971 | 18214374 | 14297505 | 11265140 | 6856125 | 3873414 | 237671 |
| 7 | 25639271 | 20099274 | 23205465 | 5979020 | 19583625 | 1865034 | 5537111 |

TABLE V.- $\alpha_{q,p,m}$

| q = 0: α | | q = 1: 2α | | q = 2: 12α | | |
|-----------------|---|------------------|---|-------------------|----|----|
| p/m | 0 | 0 | 1 | 0 | 1 | 2 |
| 1 | 1 | 1 | 1 | 5 | 8 | -1 |
| 2 | | 0 | 4 | 4 | 16 | 4 |
| 3 | | | | 9 | 0 | 27 |

| q = 3: 24α | | | | | q = 4: 720α | | | | |
|-------------------|---|----|-----|----|--------------------|------|------|-------|------|
| p/m | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 | 4 |
| 1 | 9 | 19 | -5 | 1 | 251 | 646 | -264 | 106 | -19 |
| 2 | 8 | 32 | 8 | 0 | 232 | 992 | 192 | 32 | -8 |
| 3 | 9 | 27 | 27 | 9 | 243 | 918 | 648 | 378 | -27 |
| 4 | 0 | 64 | -32 | 64 | 224 | 1024 | 384 | 1024 | 224 |
| 5 | | | | | 475 | -250 | 3000 | -1750 | 2125 |

| q = 5: 1440α | | | | | | |
|---------------------|-----|------|-------|-------|-------|------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 |
| 1 | 475 | 1427 | -798 | 482 | -173 | 27 |
| 2 | 448 | 2064 | 224 | 224 | -96 | 16 |
| 3 | 459 | 1971 | 1026 | 1026 | -189 | 27 |
| 4 | 448 | 2048 | 768 | 2048 | 448 | 0 |
| 5 | 475 | 1875 | 1250 | 1250 | 1875 | 475 |
| 6 | 0 | 4752 | -6048 | 11232 | -6048 | 4752 |

| q = 6: 60480α | | | | | | | |
|----------------------|-------|--------|--------|---------|--------|---------|--------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 19087 | 65112 | -46461 | 37504 | -20211 | 6312 | -863 |
| 2 | 18224 | 90240 | 528 | 21248 | -12912 | 4224 | -592 |
| 3 | 18495 | 87480 | 31347 | 58752 | -19683 | 5832 | -783 |
| 4 | 18304 | 89088 | 24576 | 96256 | 11136 | 3072 | -512 |
| 5 | 18575 | 87000 | 31875 | 80000 | 58125 | 28200 | -1375 |
| 6 | 17712 | 93312 | 11664 | 117504 | 11664 | 93312 | 17712 |
| 7 | 36799 | -41160 | 418803 | -570752 | 717213 | -353976 | 216433 |

TABLE VI.- $\beta_{q,p,m}$

| $q = 0: 2\beta$ | | $q = 1: 6\beta$ | | $q = 2: 24\beta$ | | |
|-----------------|---|-----------------|---|------------------|----|----|
| p/m | 0 | 0 | 1 | 0 | 1 | 2 |
| 1 | 1 | 2 | 1 | 7 | 6 | -1 |
| 2 | | 4 | 8 | 16 | 32 | 0 |
| 3 | | | | 27 | 54 | 27 |

| $q = 3: 360\beta$ | | | | | $q = 4: 1440\beta$ | | | | |
|-------------------|-----|------|-----|-----|--------------------|------|------|------|------|
| p/m | 0 | 1 | 2 | 3 | 0 | 1 | 2 | 3 | 4 |
| 1 | 97 | 114 | -39 | 8 | 367 | 540 | -282 | 116 | -21 |
| 2 | 224 | 528 | -48 | 16 | 848 | 2304 | -480 | 256 | -48 |
| 3 | 351 | 972 | 243 | 54 | 1323 | 4212 | 486 | 540 | -81 |
| 4 | 448 | 1536 | 384 | 512 | 1792 | 6144 | 1536 | 2048 | 0 |
| 5 | | | | | 2375 | 7500 | 3750 | 2500 | 1875 |

| $q = 5: 30240\beta$ | | | | | | |
|---------------------|-------|--------|--------|--------|-------|-------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 |
| 1 | 7386 | 12945 | -9132 | 5646 | -2046 | 321 |
| 2 | 17040 | 52224 | -17760 | 13056 | -4848 | 768 |
| 3 | 26568 | 94527 | -1944 | 23490 | -7776 | 1215 |
| 4 | 36096 | 136704 | 16896 | 58368 | -7680 | 1536 |
| 5 | 45750 | 178125 | 37500 | 93750 | 18750 | 4125 |
| 6 | 53136 | 233280 | 23328 | 176256 | 11664 | 46656 |

| $q = 6: 120960\beta$ | | | | | | | |
|----------------------|--------|---------|---------|--------|---------|--------|--------|
| p/m | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 28549 | 57750 | -51453 | 42484 | -23109 | 7254 | -995 |
| 2 | 65728 | 223488 | -107520 | 100864 | -55872 | 17664 | -2432 |
| 3 | 102465 | 400950 | -64881 | 170100 | -88209 | 27702 | -3807 |
| 4 | 139264 | 577536 | -9216 | 335872 | -107520 | 36864 | -5120 |
| 5 | 176125 | 753750 | 46875 | 512500 | -28125 | 57750 | -6875 |
| 6 | 212544 | 933120 | 93312 | 705024 | 46656 | 186624 | 0 |
| 7 | 257593 | 1051638 | 324135 | 585844 | 439383 | 129654 | 175273 |

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